ELEC 4700

Assignment 1

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Part 1

a. The thermal velocity is $1.8697*10^{5}$ m/s

b. The mean free path is $3.7394*10^{-8}$ m

c. i) The 2D plot of particle trajectories is shown in Figure 1 below. (N is the number of particles)

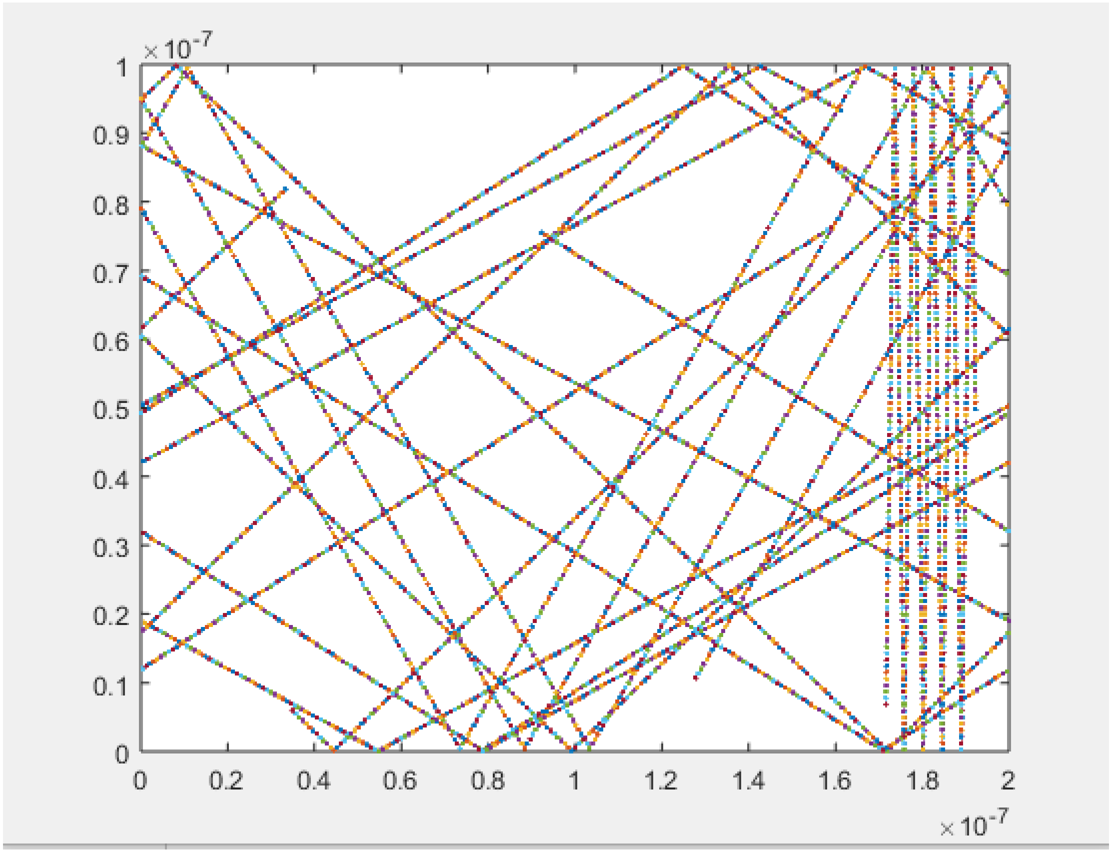

Figure 1: 2D electron trajectories without box and scattering (N=5)

ii) The temperature plot is shown in Figure 2 below

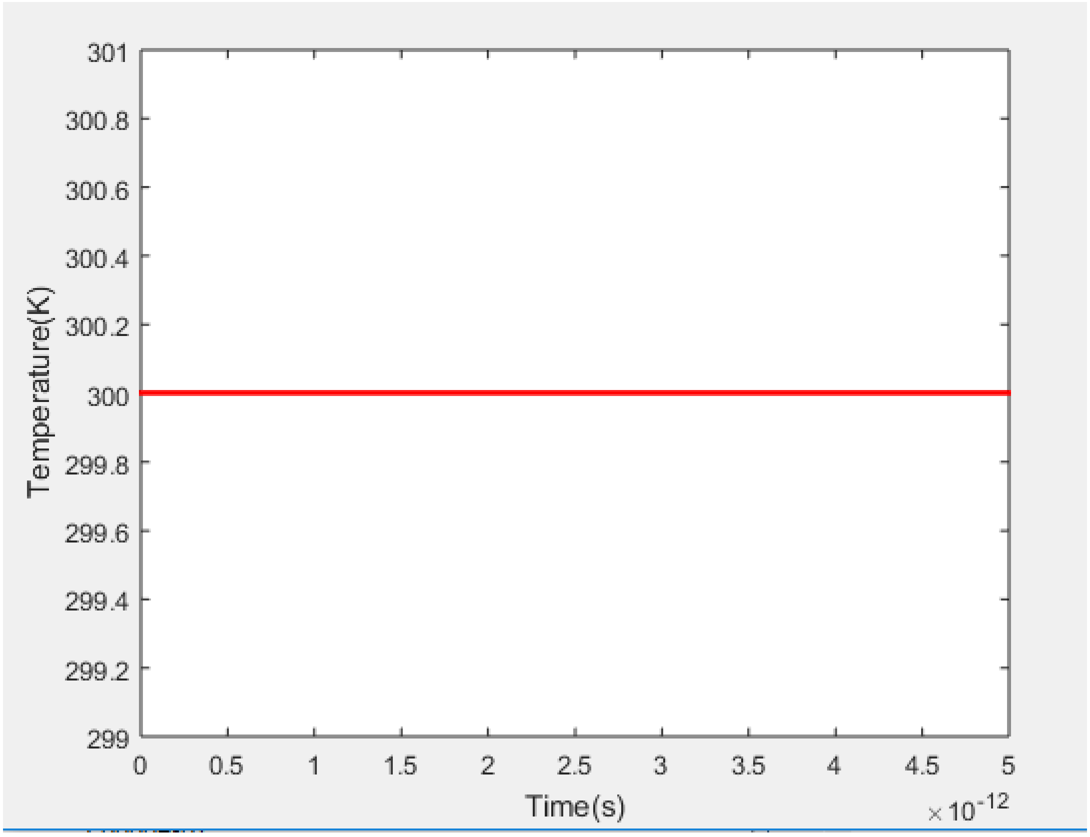

Figure 2: Temperature vs time without box and scattering

Part 2

a) The histogram of the initial velocity for each particle is shown in Figure 3.

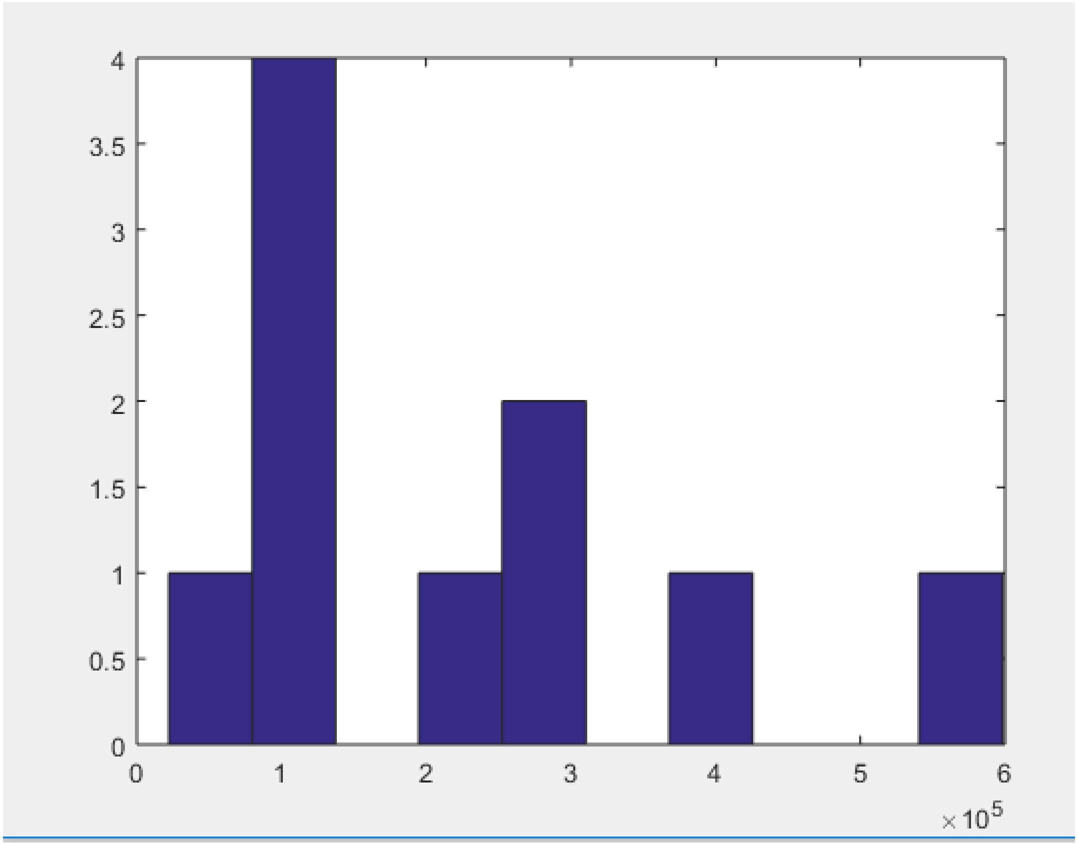

Figure 3: Histogram of initial velocity with 10 particles

b) The 2D plot of particle trajectories is given in Figure 4. (The trajectories shown in Figure 4 is actually enhanced, with box and scattering. The trajectories of electron without box can be done by getting rid of several lines of code)

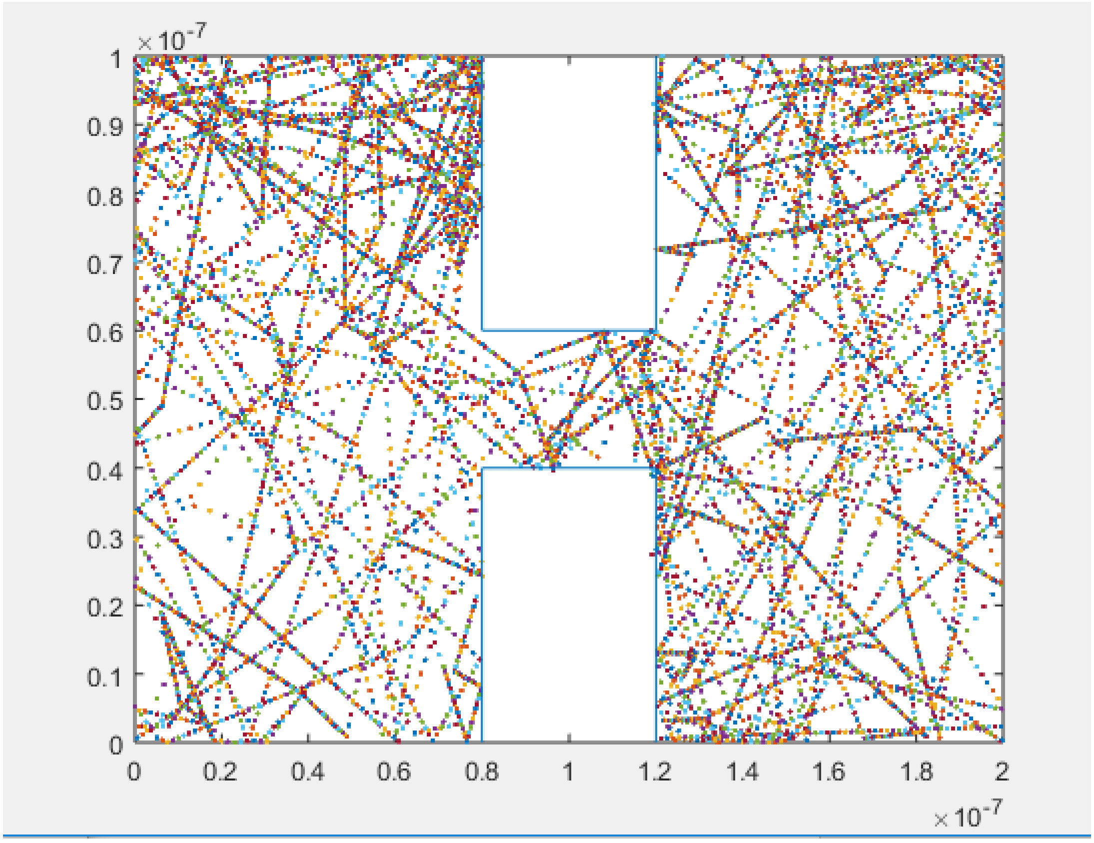

Figure 4: 2D plot of the electron trajectories with box and scattering

c) The temperature plot is shown in Figure 5.

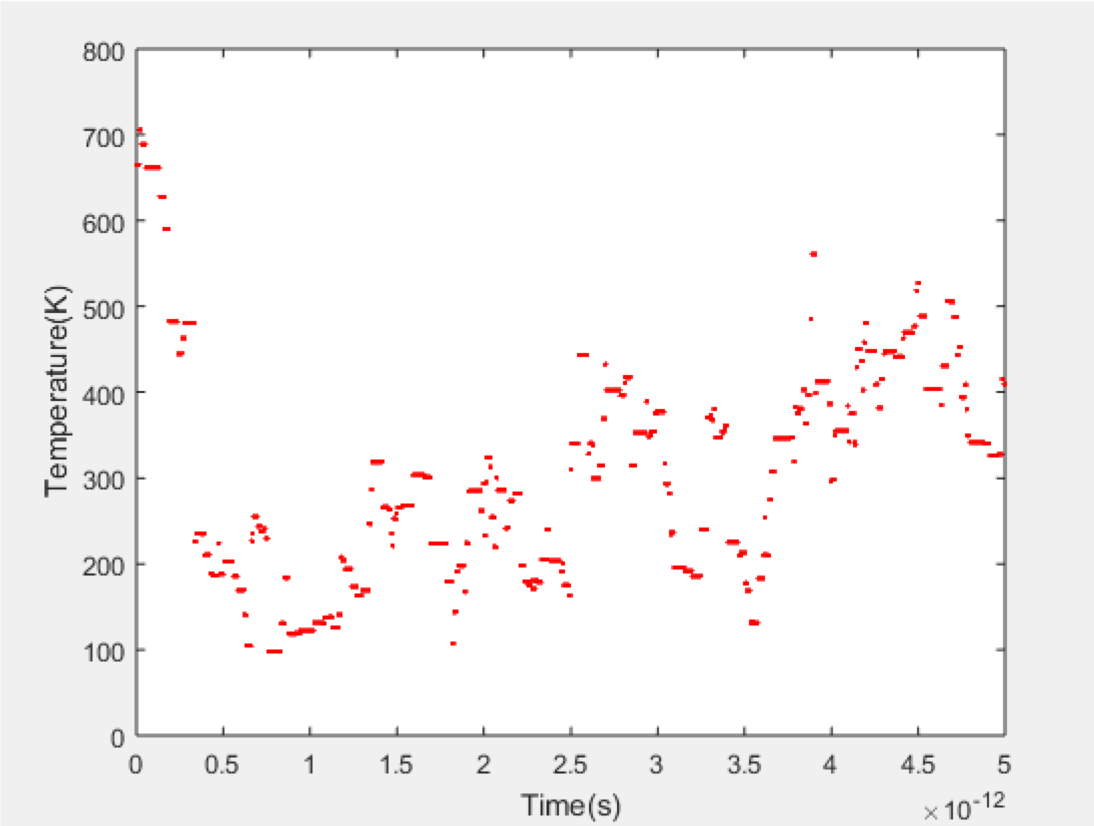

Figure 5: Temperature vs time with box and scattering

From Figure 5, we see that the average temperature of the system is around 300K. The variance is quite large, because the standard deviation of the velocity for particles is even larger than the mean velocity of the particle, which leads to significant difference between the kinetic energy of the system in each time interval. Then the temperature varies a lot.

d) The mean free path for the system with box and scattering is $1.9549*10^{-9}$ m. The mean collision time is $5.1304*10^{-15}$ s. (The mean free path and the mean collision time may not be the same for each simulation).

Part 3

a) The 2D plot of particle trajectories is shown in Figure 4.

b) The Electron density map is shown in Figure 6 and Figure 7.

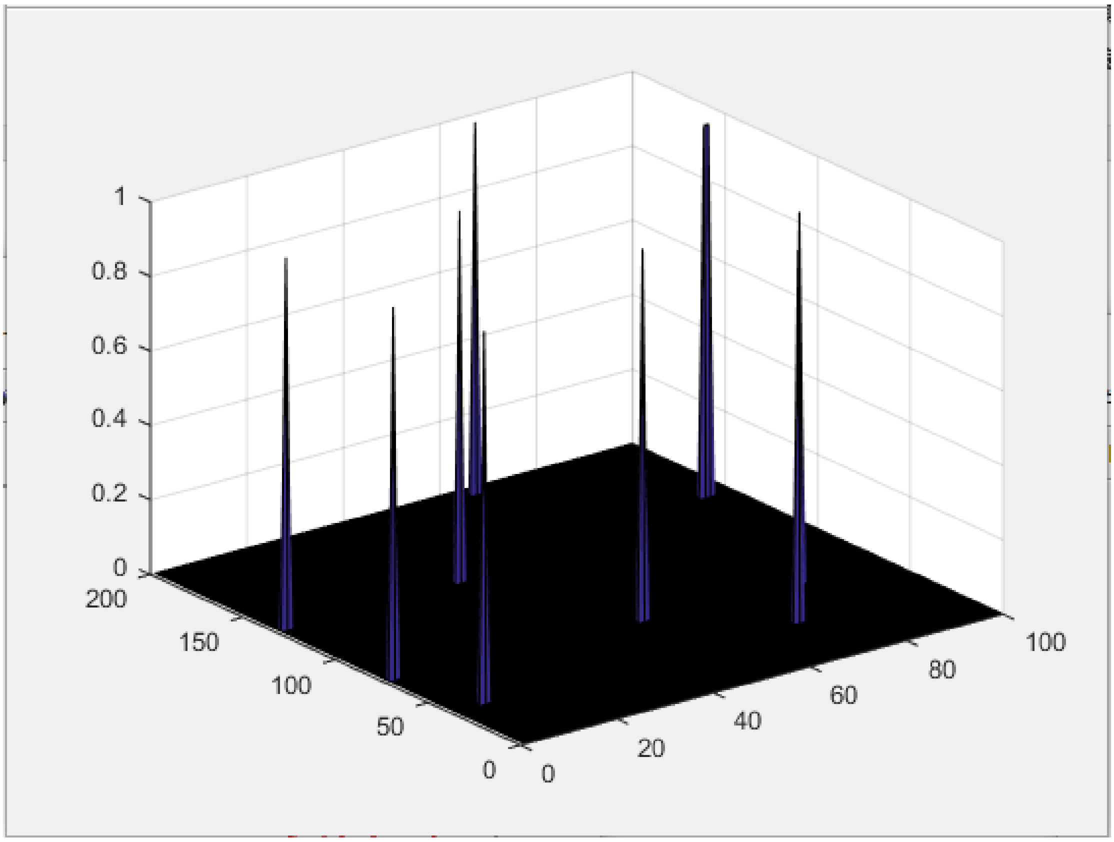

Figure 6: 3D electron density map (N=10)

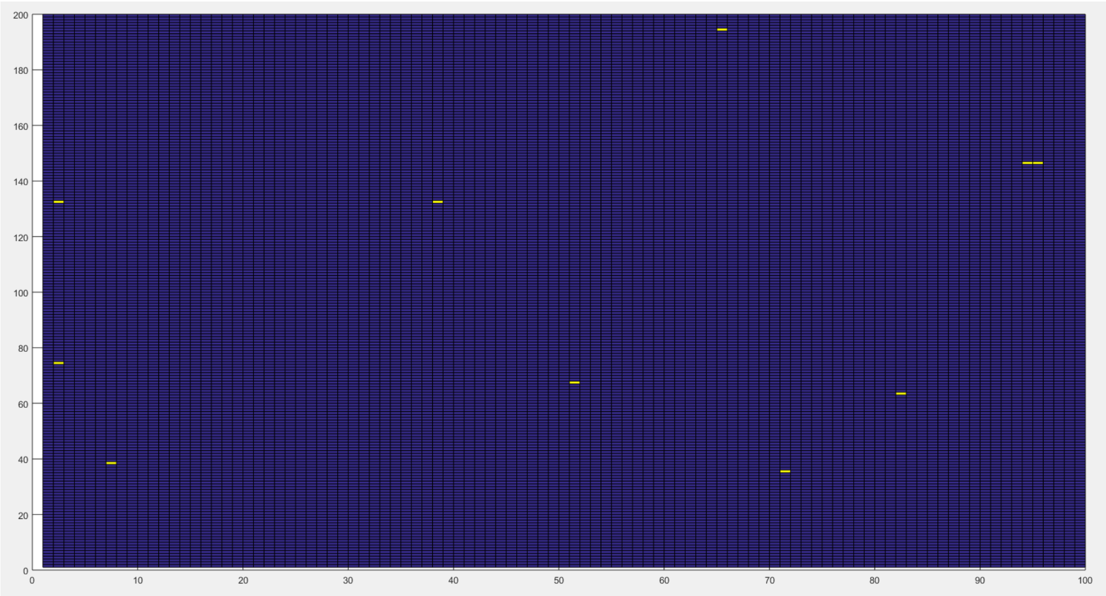

Figure 7: 2D electron density map (N= 10)

c) The temperature map is shown in Figure 8 and Figure 9.

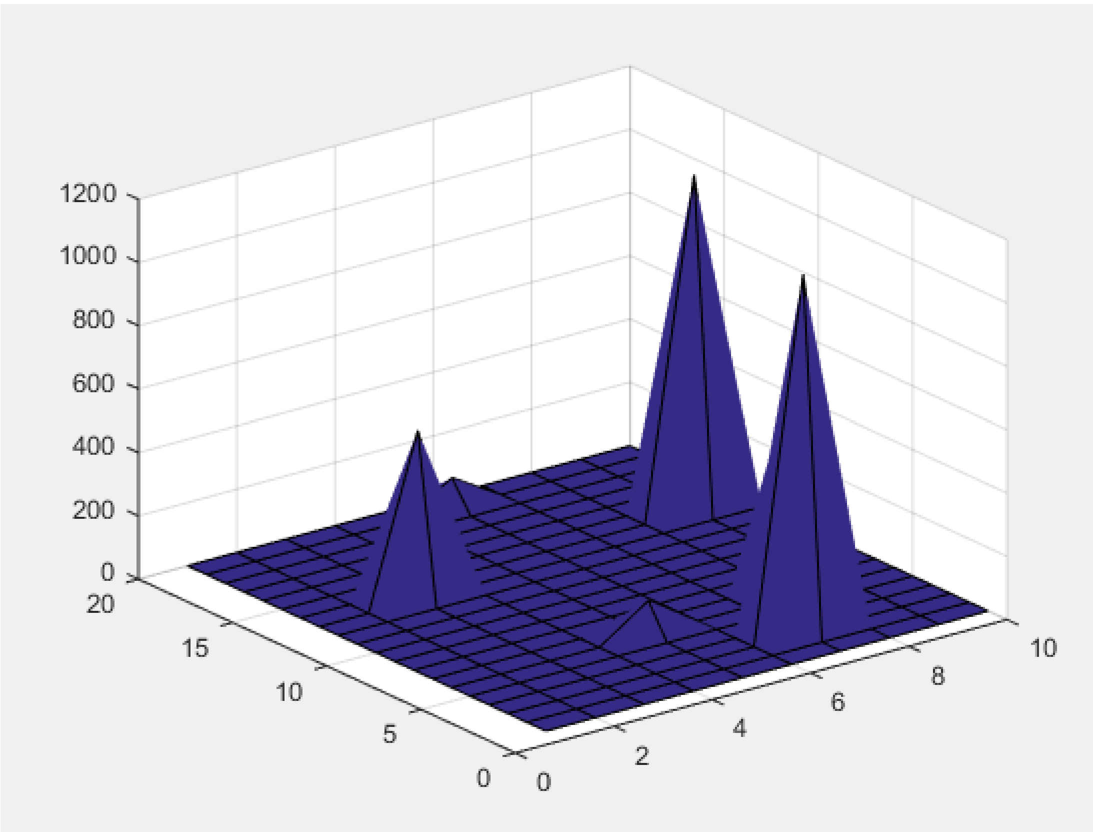

Figure 8: 3D temperature map with box and scattering

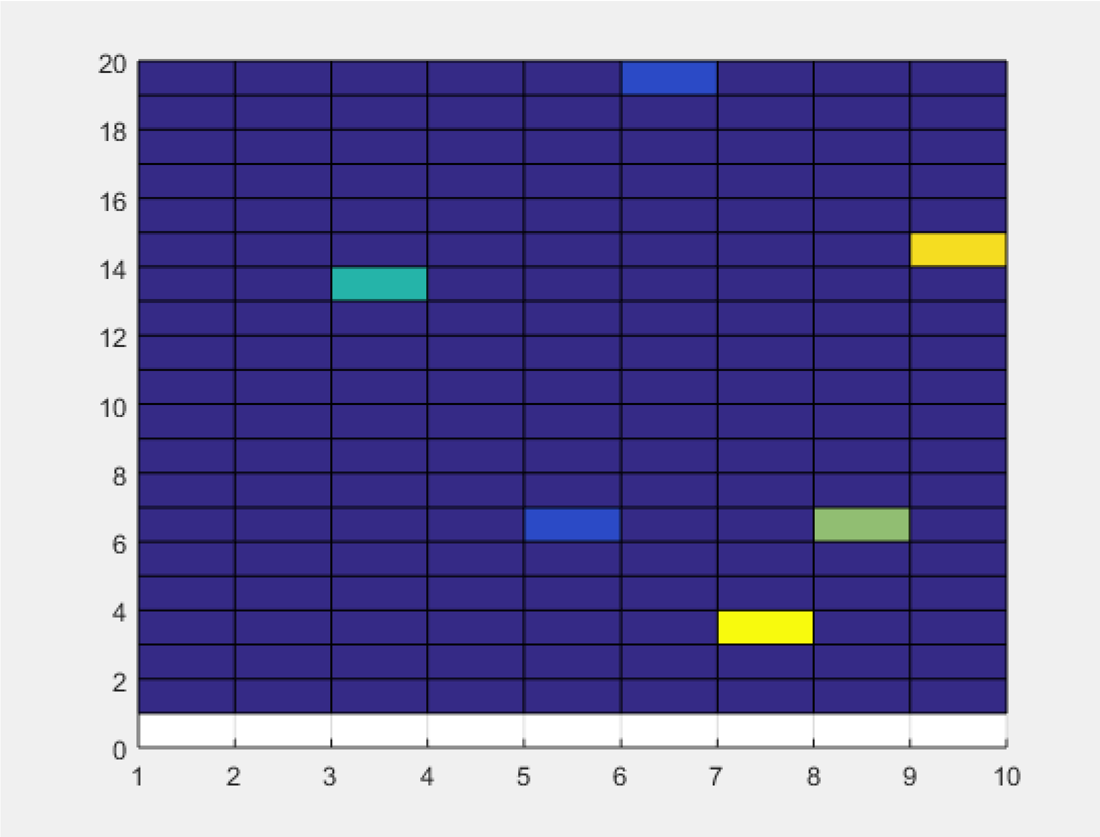

Figure 9: 2D temperature map with box and scattering

Code 1:

```
clc;
clear;

T = 300;
m0=9.11*10^-31; %in kg
W=1*10^-7;
L=2*10^-7;
mn=0.26*m0;
kB=1.38*10^-23;
tmn=0.2*10^-12;

%Part 1: question a:thermal velocity calculation
vth=sqrt(2*kB*T/mn);%thermal velocity
N=5; %number of particles
deltaT=5*10^-15;
tTotal=1000*deltaT;

%Part 1: question b: MFP
mfp=tmn*vth; %mean free path

%Initial velocity
vx=zeros(1,N);
vy=zeros(1,N);

%Initial position of each particles
xPos=zeros(1,N);
yPos=zeros(1,N);

%Initial delta position
deltaPx=zeros(1,N);
deltaPy=zeros(1,N);

%Initial angle
theta=zeros(1,N);

for i = 1:N
    x=rand*L;
    y=rand*W;
    xPos(i)=xPos(i)+x;
    yPos(i)=yPos(i)+y;
    theta(i) = theta(i) + rand*2*pi;
    vx(i)=vth*cos(theta(i));
```

```
    vy(i)=vth*sin(theta(i));
    deltaPx(i)=deltaPx(i)+vx(i)*deltaT;
    deltaPy(i)=deltaPy(i)+vy(i)*deltaT;
end


for t = 0 : deltaT : tTotal

    for i=1:N
        if yPos(i)+deltaPy(i)>W||yPos(i)+deltaPy(i)<0
            theta(i)=2*pi - theta(i);
            vy(i)=vth*sin(theta(i));
            deltaPy(i)=vy(i)*deltaT;
        end
    end

    xPos=xPos+deltaPx;
    %Periodic boundary condition in x direction
    Ix=xPos>L;
    xPos(Ix)=xPos(Ix)-L;
    Ix=xPos<0;
    xPos(Ix)=xPos(Ix)+L;


    yPos=yPos+deltaPy;
    %Boundary condition in y direction
    Iy=yPos>W;
    yPos(Iy)=yPos(Iy)-2*(yPos(Iy)-W);
    Iy=yPos<0;
    yPos(Iy)=-yPos(Iy);

    %Part 1, question c i):2-D plot of particle trajectories
    figure(1);
    plot(xPos,yPos,'.');
    hold on;
    xlim([0 L]);
    ylim([0 W]);

    KEsum=0;
    for i = 1:N
        KEsum = KEsum + (1/2)*mn*vth^2;
    end
    KEavg = KEsum /N;
    T=KEavg/kB;
```

```
    %Part 1, question c ii): Temperature plot
    figure(2);
    xlabel('Time(s)');
    ylabel('Temperature(K)');
    plot(t,T,'.r');
    xlim([0 tTotal]);
    hold on;
    pause(0.1)

end

hold off;
```

Code 2:

```
clc;
clear;

T = 300;
m0=9.11*10^-31; %in kg
W=1*10^-7;
L=2*10^-7;
mn=0.26*m0;
kB=1.38*10^-23;
tmn=0.2*10^-12;
vth=sqrt(2*kB*T/mn);%thermal velocity
N=10; %number of particles
deltaT=5*10^-15;
tTotal=1000*deltaT;

%Initial velocity
vx=zeros(1,N);
vy=zeros(1,N);

%Initial position of each particles
xPos=zeros(1,N);
yPos=zeros(1,N);

%Initial delta position
deltaPx=zeros(1,N);
deltaPy=zeros(1,N);

%Initial angle
theta=zeros(1,N);

for i = 1:N

    x=rand*L;
    y=rand*W;
    while x>0.4*L && x<0.6*L &&(y<0.4*W||y>0.6*W)
        x=rand*L;
        y=rand*W;
    end

    xPos(i)=xPos(i)+x;
    yPos(i)=yPos(i)+y;
    theta(i) = theta(i) + rand*2*pi;
```

```
    sigma = sqrt(kB*T/mn);
    vx(i) = vth/sqrt(2)*randn;
    vy(i) =vth/sqrt(2)*randn;
    v(i) = sqrt(vx(i).*vx(i) + vy(i).*vy(i));

    deltaPx(i)=deltaPx(i)+vx(i)*deltaT;
    deltaPy(i)=deltaPy(i)+vy(i)*deltaT;
end

%Part2 question a:histogram of initial velocity for each particle
figure(1);
xlabel('v(m/s)');
vAvg = mean(v);
hist(v);
xp=xPos;
yp=yPos;
vyp=vy;
vxp=vx;
xPosp=xPos;
yPosp=yPos;
dt=zeros(1,N);
sumP=zeros(1,N);
sumt=zeros(1,N);
sumNP=zeros(1,N);
sumNt=zeros(1,N);

for t = 0 : deltaT : tTotal

    dt=dt+deltaT;
    for i=1:N
        P = 1-exp(-deltaT/tmn);
        if P > rand()
            vx(i) = vth/sqrt(2)*randn;
            vy(i) =vth/sqrt(2)*randn;
            deltaPx(i)=deltaPx(i)+vx(i)*deltaT;
            deltaPy(i)=deltaPy(i)+vy(i)*deltaT;
        end
    end

    for i=1:N
        if yPos(i)+deltaPy(i)>W||yPos(i)+deltaPy(i)<0
            vy(i)=-vy(i);
            deltaPy(i)=vy(i)*deltaT;
        end
```

```
        if xPos(i)>0.4*L && xPos(i)<0.6*L
            if yPos(i)+deltaPy(i)<0.4*W||yPos(i)+deltaPy(i)>0.6*W
                vy(i)=-vy(i);
                deltaPy(i)=vy(i)*deltaT;
            end
        end
        if yPos(i)<0.4*W||yPos(i)>0.6*W
            if xPos(i)+deltaPx(i)>0.4*L && xPos(i)+deltaPx(i)<0.6*L
                vx(i)=-vx(i);
                deltaPx(i)=vx(i)*deltaT;
            end
        end

    end

    xPos=xPos+deltaPx;
    yPos=yPos+deltaPy;

    %sum of the free path for each particle
    for i=1:N
        if vx(i)~=vxp(i) || vy(i)~=vyp(i)
            FP(i)=sqrt((xPos(i)-xPosp(i))^2 + (yPos(i)-yPosp(i))^2);
            tc(i)=dt(i);
            sumP(i)=sumP(i)+FP(i);
            sumNP(i)=sumNP(i)+1;
            sumt(i)=sumt(i)+tc(i);
            sumNt(i)=sumNt(i)+1;
            dt(i)=0;
            xPosp(i)=xPos(i);
            yPosp(i)=yPos(i);
        end
    end

    %Periodic boundary condition in x direction
    Ix=xPos>L;
    xPos(Ix)=xPos(Ix)-L;
    Ix=xPos<0;
    xPos(Ix)=xPos(Ix)+L;

%     Iy=(yPos>0.6*W | yPos<0.4*W);
%     Ix=(xPos>0.4*L & xPos<0.6*L);
%     Ixy=Iy & Ix;
%
%     Ixx = xPos(Ixy)>xp(Ixy);
```

```
%   xPos(Ixx)=xPos(Ixx)-2*(xPos(Ixx)-0.4*L)
%   Ixx = xPos(Ixy)<xp(Ixy);
%   xPos(Ixx)=xPos(Ixx)+2*(0.6*L-xPos(Ixx));
%   Iyy = yPos(Ixy)>yp(Ixy);
%   yPos(Iyy)=yPos(Iyy)-2*(yPos(Iyy)-0.6*W)
%   Iyy = yPos(Ixy)<yp(Ixy);
%   yPos(Iyy)=yPos(Iyy)+2*(0.4*W-yPos(Iyy));
%
%
%
%   %Boundary condition in y direction
%   Iy=yPos>W;
%   yPos(Iy)=yPos(Iy)-2*(yPos(Iy)-W);
%   Iy=yPos<0;
%   yPos(Iy)=-yPos(Iy);

  %Part3 question a:2-D plot of particle trajectories
  figure(2);
  plot(xPos,yPos,'.');
  hold on;
  xlim([0 L]);
  ylim([0 W]);

  %block definition
  line([0.8*10^-7 0.8*10^-7],[W 0.6*W]);
  line([1.2*10^-7 1.2*10^-7],[W 0.6*W]);
  line([0.8*10^-7 0.8*10^-7],[0 0.4*W]);
  line([1.2*10^-7 1.2*10^-7],[0 0.4*W]);
  line([0.8*10^-7 1.2*10^-7],[0.6*W 0.6*W]);
  line([0.8*10^-7 1.2*10^-7],[0.4*W 0.4*W]);

  KEsum=0;
  for i = 1:N
      v_Squared = vx(i)^2+vy(i)^2;
      KEsum = KEsum + (1/2)*mn*v_Squared;
  end
  KEavg = KEsum /N;
  T=KEavg/kB;

  %Part 2, question c: Temperature plot
  figure(3);
  xlabel('Time(s)');
  ylabel('Temperature(K)');
  plot(t,T,'.r');
```

```
    xlim([0 tTotal]);
    hold on;
    pause(0.1)

    xp=xPos;
    yp=yPos;

end

%mean free path for each particle
mfp=zeros(1,N);
mtc=zeros(1,N);
for i=1:N
    mfp(i)=sumP(i)/sumNP(i);
    mtc(i)=sumt(i)/sumNt(i);
end

%Part 2, question d: MFP and tmn
%mean free path for the system
MeanFreePath = mean(mfp);
MeanCollisionTime = mean(mtc);
fprintf('Mean free path is %0.15f m\n',MeanFreePath);
fprintf('Mean collision time is %0.20f s\n',MeanCollisionTime);

%Part3 question c: electron density map
P=zeros(200,100);
xPos = xPos.*10^9;
yPos = yPos.*10^9;
for i=1:N
    for j = 1:200
        for k = 1:100
            if xPos(i) > j && xPos(i)< (j+1) && yPos(i)>k &&
yPos(i)<(k+1)
                P(j,k) = P(j,k)+1;
            end
        end
    end
end
figure(4);
surf(P);

%Part3 question d: temperature map
Temp=zeros(20,10);
xPos = xPos.*0.1;
```

```
yPos = yPos.*0.1;
for i=1:N
    for j = 1:20
        for k = 1:10
            if xPos(i) > j && xPos(i)< (j+1) && yPos(i)>k &&
yPos(i)<(k+1)
                v_Squared = vx(i)^2+vy(i)^2;
                T = (1/2)*mn*v_Squared/kB;
                Temp(j,k) = Temp(j,k)+T;
            end
        end
    end
    KE=0;
end
figure(5);
surf(Temp);

hold off;
```